of possible fragmentation processes, the consideration by MOLION of all plausible possibilities, and the structure generation capabilities of CONGEN.

We have also tried to reduce chemists' disbelief by blurring the "outsider-insider" distinction, in particular by having trained chemists work on the programs and make them useful to themselves first. Further, when "outside" chemists are first introduced to the programs, the introduction is done by another chemist who has already thought through and can readily explain many of the chemistry-related problems.

The ultimate way to counter disbelief, however, is to illustrate high levels of performance. If a potential user is aware of the goals (intent) of a program and its limitations, a few examples of results which would be extremely difficult to obtain without the program are very convincing.

The "security" of a local facility. Networking is still a relatively new concept to many people, and there is a resistance to departing from the "traditional" modes of computing. There is a sense of security in having a local computing facility with knowledgeable consultants within walking distance, and in having "hard" forms of input (eg, boxes of computer cards) and output (eg, voluminous listings). These props are difficult to simulate over a network connection - in most cases a user's interaction with the remote site takes place exclusively through a computer terminal - yet the quality of service can match or exceed that of a local facility; programs and large data sets can be entered and stored on secondary storage as can large output files; all types of program and data editing can be done with interactive editing programs; programs can be written in an interactive mode so that small amounts of control information can be input and key results output in "real time" over the terminal; And as noted in a previous section, consultation can be significantly more productive providing that the remote operating system supports the appropriate types of communication possibilities.

There can, of course, be no denying that there are problems in learning to use a distant computer system, be it for program development or for the use of certain programs. Whether or not overcoming these problems to gain access to the special resources which are available, is worth the effort, is a question answerable only by the individuals involved. Fortunately, there will always be those persons who have a pressing problem in need of solution and who are willing to try a new approach; regardless of whether or not they have had prior network experience.

The SUMEX-AIM Facility

The SUMEX-AIM computer facility consists of a Digital Equipment Corporation model KI-10 central processor operating under the TENEX time sharing monitor. It is located at Stanford University Medical Center, Stanford, California.

The system has 256K words (36 bit) of high speed memory; 1.6

million words of swapping storage; 70 million words of disk storage; two 9-track, 800 bpi industry compatible tape units; one dual DEC-tape unit; a line printer; and communications network interfaces providing user terminal access via both TYMNET and ARPANET.

Software support has evolved, and will continue to evolve, based on user research goals and requirements. Major user languages currently include INTERLISP, SAIL, FORTRAN-10, BLISS-10, BASIC and MACRO-10. Major software packages available include OMNIGRAPH, for graphics support of multiple terminal types, and MLAB, for mathematical modelling.

The SUMEX-AIM computer generally is left with no operator in attendance; thereby helping to eliminate some overhead, but also creating some problems. Users who wish to run jobs requiring tapes must make arrangements to mount their own tapes. Likewise, obtaining listings from the line printer can be somewhat difficult since there is no regular schedule for distribution of this output. The solution to these two problems has been to make keys to the machine room available at strategic locations, convenient to all groups of local users. This experiment in basic "resource sharing" has not resulted in any of the major problems one might expect from having a fairly large group of people with hands-on access to a computer.

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Figure Captions

Figure 1. Interactions in the SUMEX-AIM community

Figure 2. Access to SUMEX-AIM

Figure 3. Total ion current vs. spectrum number in a GC/LRMS run

Figure 4. The spectrum corresponding to scan 492 in Figure 3. (top) Raw data. (bottom) Output from CLEANUP

Figure 5. Low resolution mass spectrum of unknown X. The indicated superatoms were deduced from the spectrum and a knowledge of the chemical history of the sample. With these and other constraints, CONGEN obtained the indicated results.

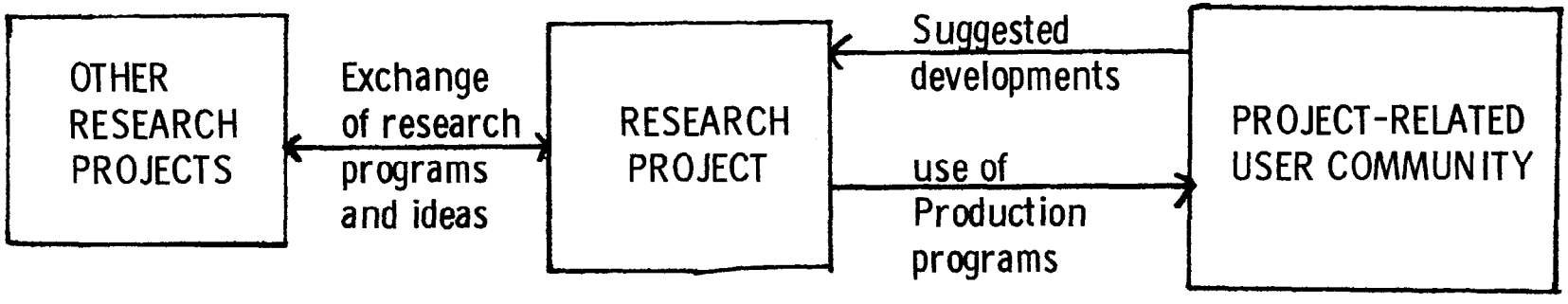

OTHER
RESEARCH
PROJECTS
Exchange
of research
programs
and ideas
RESEARCH
PROJECT
Suggested
developments
use of
Production
programs
PROJECT-RELATED
USER COMMUNITY

Fig. 1

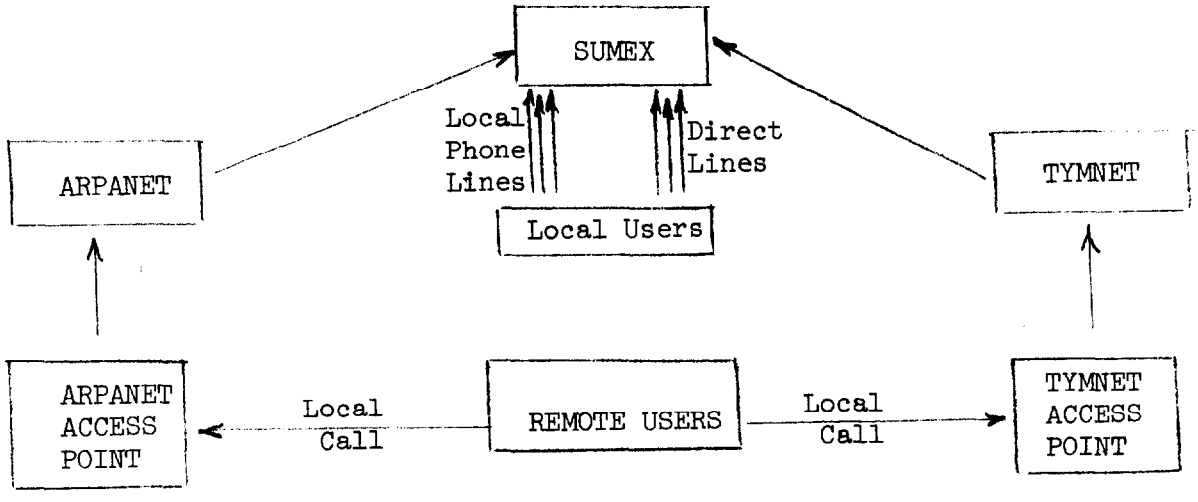


Fig. 2.

Figure 3. GC Trace (to be supplied)

Figure 4. Two Mass Spectra (to be supplied)

Figure 5. Mass Spec of Unknown (to be supplied)

Figure 3

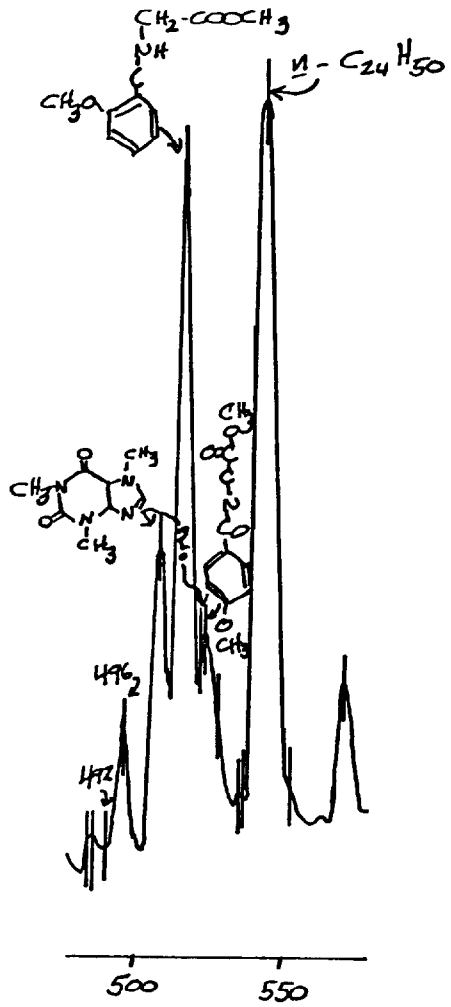
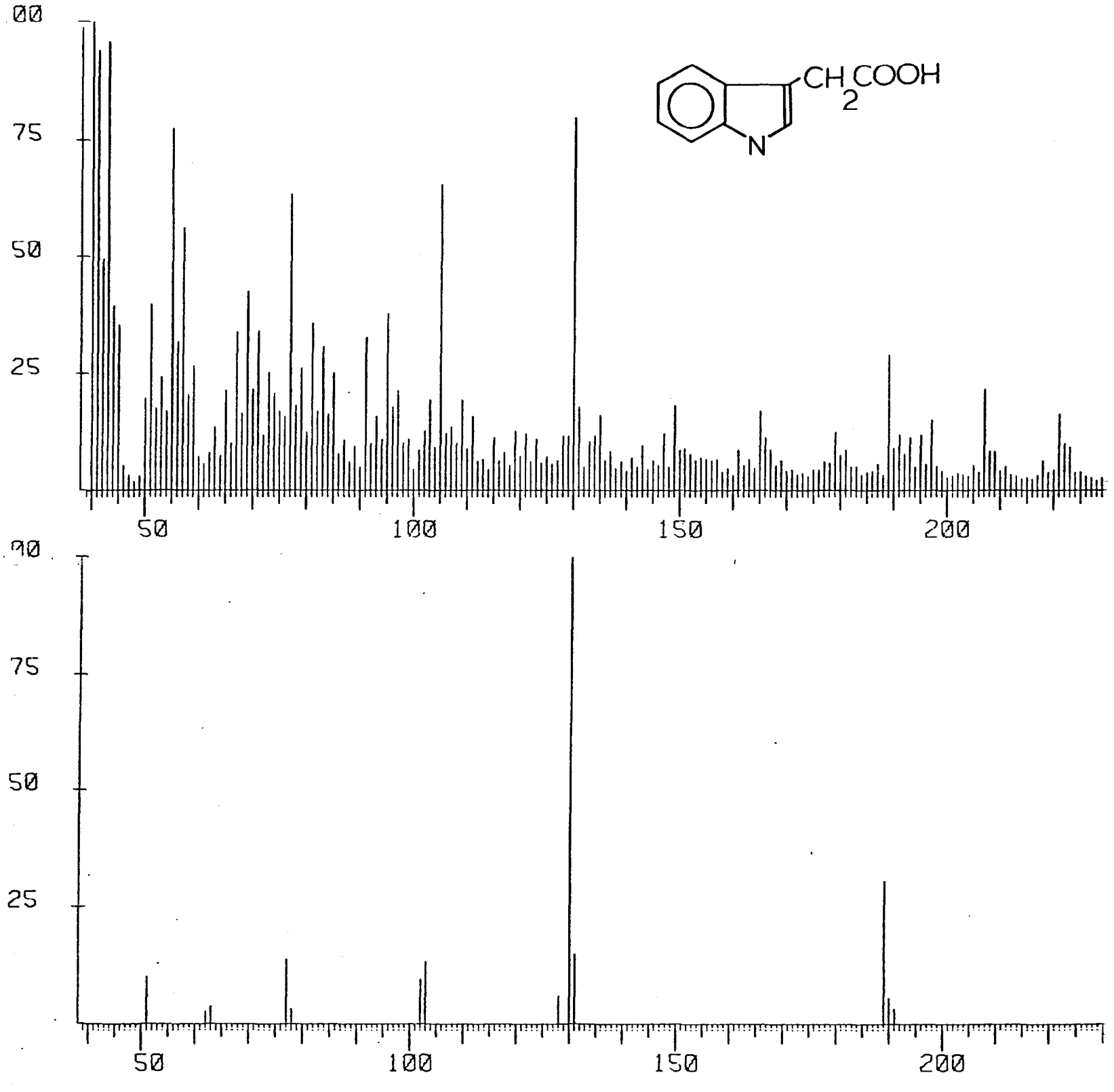
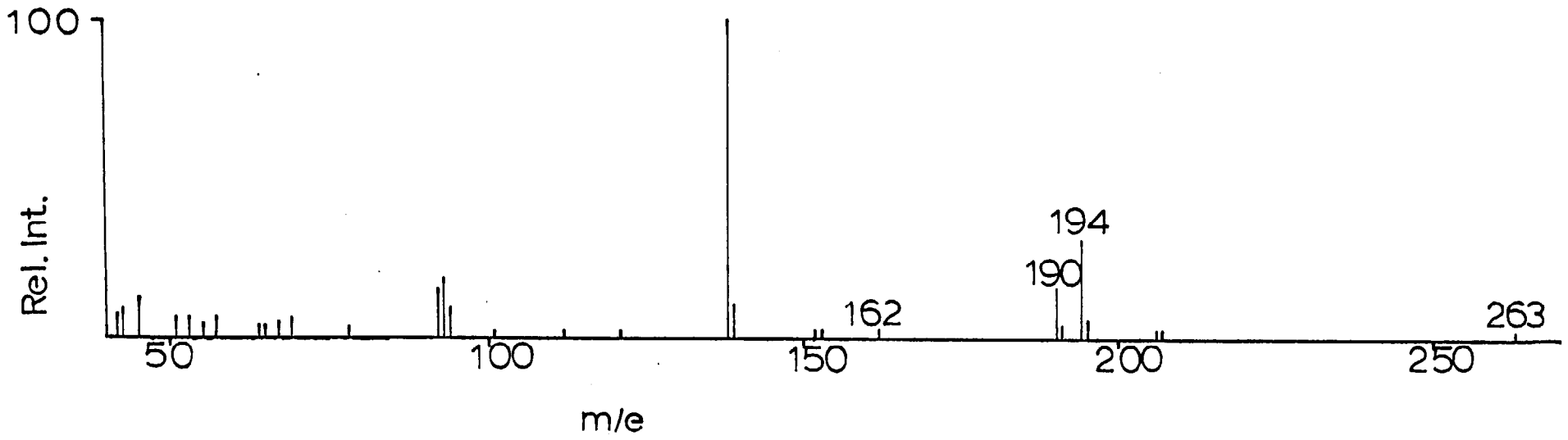


Figure 4



CLEAN SPECTRUM
EXP. W247 20-DEC-74
SPECTRUM NO. 492

Figure 5

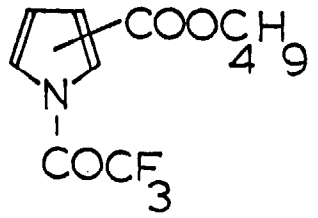


SUPERATOMS

$\underline{n}$-C_4H_9OOC- 1

CF_3CO- 2

CONGEN RESULT



3

The undersigned agrees to accept responsibility for the scientific and technical conduct of the project and for provision of required progress reports if a grant is awarded as the result of this application.

5/7/75
Date

Principal Investigator or
Project Director

II.B. SUMMARY OF RESOURCE USAGE

The outside uses of our resource-related research are listed in Part III of the Description of Progress (section II-A).

II.C. RESOURCE RELATED RESEARCH EQUIPMENT LIST

EQUIPMENT SUMMARY

1)	MM11-U Memory Module PDP 11/45 CM Central Processor (Ser. 5200) FP11-B Floating Point Processor TM11-EA Nine Channel Magnetic Tape Drive and Controller	$45,372
2)	Systems Industries PDP Model 20 or 45 compatible disk system Model 3040 Controller Daisy Chain Option Certified Disk Pack	11,622
3)	GT 40AA Display System 115V	14,359
4)	M792 32 word Diode Memory for PDP 11 (4)	1,359
5)	Disk Pack	268
6)	E-30-2004 RB Bud Cabinet	322
		$73,302

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III. RESOURCE FINANCES

A. SUMMARY OF EXPENDITURES

B. DETAILS

C. SUMMARY OF RESOURCE FUNDING

D. BUDGET EXPLANATION/JUSTIFICATION

SECTION II—BUDGET (USUALLY 12 MONTHS)	FROM	THROUGH	GRANT NUMBER
	8/1/75	7/31/76	RR612-05A1

A. ITEMIZE DIRECT COSTS REQUESTED FOR NEXT BUDGET PERIOD

PERSONNEL NAME (Last, First, Initial) (a)	TITLE OF POSITION (b)	TIME OR EFFORT %/HRS. (c)	SALARY REQUESTED (d)	FRINGE BENEFITS (See Instructions) (e)	TOTAL (f)
	PRINCIPAL INVESTIGATOR				
See separate listing					
	Subtotals →		$	$	

(Indicate cost of each item listed below) — TOTAL (Columns (d) and (e)) → $ 207,822

CONSULTANT COSTS (See Instructions) $ 0

EQUIPMENT PDP-11 Maintenance Contract - $8,800
MAT-711 Maintenance - $7,000 $ 15,750

SUPPLIES Office supplies (500), electronics supplies (1000), GC supplies (1100), liquid nitrogen (1100), chemicals and etc. (1600), data recording media (1100), minicomputer supplies (750) $ 7,150

TRAVEL
DOMESTIC 2 East Coast and 2 West Coast trips $ 1,400
FOREIGN $ 0

PATIENT COSTS (See instructions) $ 0

ALTERATIONS AND RENOVATIONS $ 0

OTHER EXPENSES (Itemize)
Telephone (office & data) - 1800
Terminal & communication equipment lease - 5240
Publications, etc. - 1800 $ 8,840

TOTAL DIRECT COST (Enter on Page 1, Item 10) $ 240,962

INDIRECT COST (See Instructions)
47 % S&W* NTDC
Date of DHEW Agreement: July 30, 1973
☐ Not Requested
☐ Under negotiation with:
*If this is a special rate (e.g. off-site), explain.

SECTION III—FISCAL DATA FOR CURRENT BUDGET PERIOD (USUALLY 12 MONTHS)	FROM	THROUGH	GRANT NUMBER
	5/1/74	7/31/75	R 24 RR00612-05A1

The following pertains to your CURRENT PHS budget. Do not include cost sharing funds. This information in conjunction with that provided on Page 2 will be used in determining the amount of support for the NEXT budget period.

A. BUDGET CATEGORIES		CURRENT BUDGET (As approved by awarding unit) (1)	ACTUAL EXPENDITURES THRU 3/31/75 (Insert Date) (2)	ESTIMATED ADDITIONAL EXPENDITURES AND OBLIGATIONS FOR REMAINDER OF CURRENT BUDGET PERIOD (3)	TOTAL ESTIMATED EXPENDITURES AND OBLIGATIONS (Col. 2 plus Col. 3) (4)	ESTIMATED UNOBLIGATED BALANCE (Subtract Col. 4 from Col. 1) (5)
Personnel (Salaries)		194,183	122,728	71,455	194,183	0
Fringe Benefits - included in personnel (salaries)						-
Consultant Costs		-	-	-	-	-
Equipment		105,050	92,510	10,715	103,225	1,825
Supplies		12,000	4,240	2,000	6,240	5,760
TRAVEL	Domestic	2,700	242	2,500	2,742	0
	Foreign	-	-	-	-	-
Patient Costs		-	-	-	-	-
Alterations and Renovations		-	-	-	-	-
Other		10,000	15,639	1,904	17,543	(7,543)
Total Direct Costs		323,933	235,359	88,574	323,933	0
Indirect Costs (If included in award)		114,531	76,167	38,364	114,531	0
TOTALS →		$438,464	$311,526	$126,938	$438,464	$ 0

Use space below to:

B. List all items of equipment purchased or expected to be purchased during this budget period which have a unit cost of $1000 or more.

C. Explain any significant balance or deficit shown in any category of Column 5.

D. List all other research support for Principal Investigator by source, project title, and annual amount.

DETAILED SALARY DATA
NIH GRANT RR 612-05A1
8/1/75-7/31/76

	% Effort	Salary	Fringe Benefits	Total
PRINCIPAL INVESTIGATORS:				
C. Djerassi	10	0	0	0
J. Lederberg	10	0	0	0
E. Feigenbaum	10	2,737	520	3,257
RESEARCH ASSOCIATES				
D. Smith	100	20,179	3,834	24,013
R. Carhart	100	18,783	3,569	22,352
H. Brown	100	20,179	3,834	24,013
G. Dromey	100	18,139	3,447	21,586
A. Duffield	15	3,784	718	4,502
PROGRAMMERS:				
W. White	50	9,177	1,744	10,921
G. Jirak	100	12,418	2,360	14,778
K. Stone	50	6,440	1,224	7,664
ELECTRONICS ENGINEER:				
N. Veizades	50	11,270	2,141	13,411
ELECTRONICS TECHNICIAN:				
D. Pearson	50	7,226	1,373	8,599
SENIOR RESEARCH ASSISTANT:				
A. Wegmann	100	17,350	3,297	20,647
RESEARCH ASSISTANTS:				
M. Stefik	100	5,528	1,050	6,578
P. Friedland	100	5,528	1,050	6,578
K. Morrill	100	3,420	650	4,070
SECRETARIAL SUPPORT:				
G. Perry	50	5,693	1,083	6,775
D. Larson	50	5,581	1,061	6,642
M. Allen	10	1,206	229	1,435
TOTAL:		$174,638	$33,184	$207,822

III.C. SUMMARY OF RESOURCE FUNDING

The interdisciplinary resource-related research project is almost wholly funded by the Biotechnology Resources Branch of the NIH. Computing support is provided by the NIH-funded SUMEX computer facility at Stanford (NIH Grant #RR00785-02, Professor Joshua Lederberg, Principal Investigator).

Additional support for chemistry research related to this grant is provided by NIH Grants GM-06840 and AM-04257 (Professor Carl Djerassi, Principal Investigator).

BUDGET JUSTIFICATION

Personnal remains the same as justified in the renewal application report with the exception of the substitution of Dr. Raymond Carhart for Dr. Natesa Sridharan. Salaries are increased by 9% per year and staff benefits are computed at 18% for the period 9/74-8/75, and are increased 1% per year thereafter, based on current University projections. Other budget categories are increased by 10% per year to account for inflation.

Equipment maintenance is budgeted for the proposed stand-alone PDP-11 system under DEC contract based on current prices. Also included is a budget for maintenance of the MAT-711 system. This estimate is based on our experience with parts replacements to date. We will provide the necessary manpower because Varian cannot provide adequate service.

Supplies are budgeted in various categories based on our operating experience to date. Electronics supplies include parts necessary for maintaining our electronics and test equipment. GC supplies include carrier gases, columns, phases, syringes, septa, etc., for GC/MS operation. The liquid nitrogen is required for cold trap operation on the MAT-711. Chemicals, glassware, etc., include the various organic chemicals, glassware, apparatus, glass tubing, etc. needed to support the recording paper for the calcomp paper and pens for ion currennt and spectrum plotting. Mini-computer supplies include paper, magnetic tape, ribbons, spare disk cartridges, etc., for data system operation.

The travel budget covers estimated needs (2 east coast and 2 west coast) trips for attending related professional meetings and interfacing potential program users nationally. No foreign travel is budgeted.

The "Other" budget includes operating telephone, office supplies, postage, reproduction, etc., support necessary for this project based on our previous experience. Terminal rental covers four terminals to be distributed among the MS laboratory, the Computer Science Department, and J. Lederberg's laboratory.

IV. DETAILED DESCRIPTION OF RESOURCE PROJECTS

Projects using the structure elucidation tools developed under this resource related research grant are listed in the Description of Progress (section II-A).